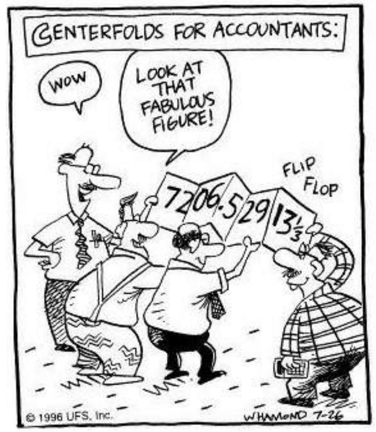
Chemistry BC2001x: Lab Lecture Week 2

- **Math with significant figures**
- **When to round?**
- **Uncertainties**
  - **Absolute**
  - **Relative**
- **Math with uncertainties**



Arithmetic involving Significant Figures

RULE 1

- **In addition and subtraction the result is written with the uncertain digit in the same *decimal place* as the term whose uncertain digit is in the earliest *decimal place.***

Note: **The decimal place of an uncertain digit may fall before or after the decimal point.**

Addition/subtraction with Significant Figures

Example 1:

Suppose a Celsius temperature is given as 37°C. What is T (K)?

T(K)= T(°C) + 273.15 [exact]

In what decimal place is the uncertainty of 37°C ?

Does 273.15 have an uncertainty?

In what decimal place is the uncertainty of the sum?

T (K) = 37 + 273.15 = 310.15 K

What is correctly rounded T in K? → 310 K

Addition/subtraction with Significant Figures

Example 2: $2.79 \times 10^4 - 7.8 \times 10^2 = 27120$

How should this answer be written?

Which digit is uncertain?

It helps to write in simple decimal form:

$$\begin{array}{r} 27900 \\ -\underline{\quad 780} \\ 27120 \end{array}$$

$\rightarrow 2.71 \times 10^4$

Conclusion: be careful when added terms are written with different powers of ten.

Writing answers with correct number of significant figures

```
      14.452
       1.5
+      0.26
```

- Round to what decimal place?
- **uncertainty of 14.452 is in third decimal place (thousandths)**
- **uncertainty of 1.5 is in the first decimal place (tenths)**
- **uncertainty of 0.26 is in second decimal place (hundredths)**
- **Uncertainty of sum is in which decimal place?**

When to Round?

14.452 + 1.5 + 0.26 = ?

Round when? Two possibilities:

- **Round first, then add:**
  14.5 + 1.5 + 0.3 = 16.3 **…or**
- **Add first, then round:**
  14.452 + 1.5 + 0.26 = 16.212 → 16.2
- **The second is correct:**
  avoids ROUNDOFF ERROR.

Arithmetic with Significant Figures

RULE 2

In multiplication and division the result has same number of significant figures as the term with the fewest significant figures.

Multiplication/division with Significant Figures

Example 1:

How may moles of carbon in 5.53 g?

moles = (grams)/(atomic weight)

= (5.53 g)/(12.011 g/mole)

= 0.46041129 moles..

How many significant figures?
What is correctly rounded result?

→ 0.460 moles

Multiplication/division with Significant Figures

Example 2:

- $\frac{(0.082057)(298.15)(0.3970)}{(0.94)(24.586)}$
- = 0.420266937 → _____
- What is correctly rounded result?
- 0.42
- It is good practice to write the UNROUNDED result first, then the rounded. The unrounded value is used in any subsequent calculations.

Absolute Uncertainties

- For any experimental value X, there is an absolute uncertainty, ΔX
- ΔX has the same units as the value:
  62 ± 4 pounds (write the units once)
- ΔX is by convention written with one non-zero digit when reporting final results
- The value X should be rounded to the same decimal place.
  0.4764 ± 0.0003 grams

Relative uncertainties

- Definition: relative uncertainty
  = (absolute uncertainty) / (value)
  Relative uncertainty = ΔX/X
- Technically have one (non-zero) significant digit, but we often keep two in intermediate steps to avoid roundoff error.
- Final answers generally reported with their absolute uncertainties (relative uncertainties used in intermediate steps).

Relative Uncertainties

- relative uncertainty
  = (absolute uncertainty)/(value)
- Units?
- May be reported as decimal fraction, often as a %, or parts per thousand (ppt):
- relative uncertainty 0.003 = 0.3% = 3 ppt

Absolute uncertainties
Where do you find them?

When you look up data:

- sometimes an explicit uncertainty is given (check table headings and footnotes!)
- If not, you may assume ±1 in the rightmost digit reported.

Absolute uncertainties
when you look up data

- **Atomic weight of Titanium?**
  Look at Periodic table: 47.88†
  Read the footnote:
  " †These weights are considered reliable to ±3 in the last place."
  result: ____________________
- **Density of ethanol at 25°C**
  from table: 0.794 g/mL
  result: ____________________

Absolute uncertainties
when you look up data

- Numbers are sometimes written in the form 1.00794(7) g/mol
- Frequently seen in tabulations
- The value in parentheses is the uncertainty associated with the last digit
- Atomic weight of H listed above is
  1.00794 ± 0.00007 g/mol

Absolute uncertainties
Where do you find them?

When you are collecting the data in lab

- This is an important part of making the measurement
- It depends on the equipment and on you
- You must learn to make estimates
- We will spend time on this in lab

Propagating uncertainties

- How do we account for the cumulative effect of multiple uncertainties?
- We propagate the uncertainties..

Example: Common laboratory procedure: weigh by difference:

- bottle + sample: 37.5 ± 0.3 g
  empty bottle: 21.3 ± 0.3 g
  weight of sample: 16.2 ± ? g
- What is the uncertainty of the result?

Propagating uncertainties

- We will make a cautious "worst-case scenario" estimate.
- How wrong could the result be if the uncertainties all worked against us?
- Two extremes: 37.5- 21.3 = 16.2
  - (37.5 + 0.3) - (21.3 - 0.3) = 37.8 - 21.0 = 16.8
    this is 0.6 larger than the original result.
  - (37.5 - 0.3) - (21.3 + 0.3) = 37.2 - 21.6 = 15.6
    this is 0.6 smaller than the original result.
- Conclusion: 16.2 ± 0.6 g

Propagating uncertainties in addition and subtraction

Algebraically: $C = A + B$

If A has uncertainty ΔA, and B has uncertainty ΔB, then

$(C + \Delta C) = (A + \Delta A) + (B + \Delta B)$ so

$$\Delta C = \Delta A + \Delta B$$

The general rule is

When adding or subtracting, the absolute uncertainty of the result is the sum of the absolute uncertainties of the values.

Propagating uncertainties in multiplication and division

Algebraically: $C = AB = A \times B$

$(C + \Delta C) = (A + \Delta A) \times (B + \Delta B)$

$= AB + B\,\Delta A + A\,\Delta B + \Delta A\,\Delta B$

$\Delta C = B\,\Delta A + A\,\Delta B + \Delta A\,\Delta B$

Uncertainties are small. The last term, the product of two small terms, is very small: it can be ignored.

Divide both sides by C (or equivalently AB):

$\Delta C/C = B\,\Delta A/AB + A\,\Delta B/AB = \Delta A/A + \Delta B/B$

The general rule is:

When multiplying or dividing, the relative uncertainty of the result is the sum of the relative uncertainties of the values.

Propagating uncertainties
in multiplication and division

- What about multiplying by a constant?
- Suppose $y = ax$ where a is an exact constant.
- If the constant has an uncertainty, the general rule still holds,
- If the constant has zero uncertainty:

  $(\Delta y/y) = (\Delta x/x)$ same relative uncertainties

  $\Delta y = y\,(\Delta x/x)$

  $= ax\,(\Delta x/x) = a\Delta x$
- Conclusion: if $y = a\,x$ then $\Delta y = a\,\Delta x$

Propagating uncertainties
in multiplication by a constant

Rule: If $y = ax$, where a is exact, then $\Delta y = a\Delta x$

Example: 167 ± 1 cm = ? inches

1 inch = 2.54 cm (exactly)

(167 cm)/(2.54 cm/in) = 65.7480 inch

(1 cm)/(2.54 cm/in) = 0.3937 inch

correctly rounded result: ___________

The absolute size of the uncertainty doesn't change when the units change (but the numerical value does!)

Estimation of maximum uncertainty or uncertainty analysis

- Many chemistry lab calculations involve numerous multiplications and divisions.
- We will use a systematic tabular method to propagate the estimated uncertainties of all quantities in the calculation to get the estimated uncertainties of the final result.
- Very important in assessing precision, and thinking about experimental design.

Propagating uncertainties
systematically in lab reports

1) convert absolute uncertainties to relative uncertainties for all quantities involved in the calculation (keeping an extra digit to avoid roundoff error)
2) If the operations combining these values involve multiplications and/or divisions only, then the sum of the relative uncertainties gives the relative uncertainty of the result
3) multiply this relative uncertainty by the calculated result (the value) to get its absolute uncertainty.
4) Round the final absolute uncertainty to one digit.
5) Round the value to the same decimal place.

Lab use first in Gravimetric Experiment ….